

# A Simple Kriging Method Incorporating Multiscale Measurements<sup>1</sup>

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<sup>1</sup> Received:                      Accepted:

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Suggested Running Head: Multiscale Simple Kriging

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## ABSTRACT

In this study, we propose a kriging algorithm to incorporate data observed at multiscales (multi-resolutions). We assume that there are a number of measurements at different scales, and that the target scale at which the parameter values are needed may be different from the measurement scales. Several synthetic examples has been used to illustrate the method. These examples demonstrate that, by incorporating measurements from all scales, the estimated field is better than the field estimated using measurements from any individual scale. This method also allows us to estimate a parameter field at the scale that does not have any measurements.

*KEYWORDS:* kriging, simple kriging, multiscale, multiresolution

## Introduction

Kriging has been widely used to incorporate spatially sampled data and estimate the conditional mean field and its associated (co-)variance [*Journel and Huijbregts*, 1978; *Clark*, 1979; *Kitanidis*, 1997; *Deutsch and Journel*, 1998]. Although in many applications the data may be sampled at different scales (resolutions) and quite often these scales are different from the scale at which estimates are needed, data are usually used in kriging as if they were sampled at the scale of numerical grids. In addition, in some applications, for example, adaptive mesh refinement, one may need to assign parameter values at a different resolution based on parameter values at the existing resolutions. This calls a methodology to assign parameter values across different scales. Few studies investigated the effect of multiscale data on the estimated field. Kupfersberger et al. (1998) studied multiscale cokriging with a primary attribute and a second attribute, where the second attribute is available at a large scale and the primary attribute is measured at the modeling scale. The measurements of the second attribute at large scale are used to improve the estimate of the primary attribute.

In this research, we assume that the parameter of interest is measured at several different scales (resolutions). Our aim is to estimate the conditional mean field and conditional covariance of the parameter at a target scale, which may be different from measurements scales and measurements may not be available at this target scale.

The paper is organized as follow. In section 2, we first formulate the kriging estimate using all measurements at different scales. The covariance functions across different scales that are required in the kriging system are given in Section 3. The method is then demonstrated using a few synthetic examples, followed by a short summary.

## Multiscale Simple Kriging

Let  $Y$  be a second-order stationary random function (say, the log hydraulic conductivity) defined on domain  $\Omega$ , characterized by the mean  $\langle Y \rangle$  and the unconditional covariance function  $C_Y(\mathbf{x}, \mathbf{y})$ , for  $\mathbf{x}, \mathbf{y} \in \Omega$ . Suppose that we have observed  $Y(\mathbf{x})$  at  $K$  different scales (resolutions)  $S_1, S_2, \dots, S_K$ , and that there are  $N_k$  measurements at scale  $S_k$ , observed at locations  $\mathbf{x}_i^{(k)}$ ,  $i = \overline{1, N_k}$  and  $k = \overline{1, K}$ . For any  $\mathbf{x}$  at the scale  $S_0$  that may be different from the observation scales  $S_k$ ,  $k = \overline{1, K}$ , the kriging estimation may be written as a linear combination of all available measurements,

$$Y^{(0)}(\mathbf{x}) = \sum_{k=1}^K \sum_{i=1}^{N_k} \alpha_i^{(k)}(\mathbf{x}) Y^{(k)}(\mathbf{x}_i^{(k)}), \quad (1)$$

where coefficients  $\alpha_i^{(k)}(\mathbf{x})$  are determined by minimizing the estimate errors at the ensemble sense, which yields the kriging equations

$$\sum_{k=1}^K \sum_{i=1}^{N_k} \alpha_i^{(k)}(\mathbf{x}) C_Y^{(k,n)}(\mathbf{x}_i^{(k)}, \mathbf{x}_j^{(n)}) = C_Y^{(0,n)}(\mathbf{x}, \mathbf{x}_j^{(n)}), \quad n = \overline{1, K}, j = \overline{1, N_n} \quad (2)$$

where  $C_Y^{(k,n)}$  is the covariance function between scales  $S_k$  and  $S_n$ , and  $C_Y^{(0,n)}$  is covariance between scales  $S_n$  and  $S_0$ , which is the scale of being estimated. There are  $N = \sum_{k=1}^K N_k$  linear equations and  $N$  unknowns in Equation (2). Note that the coefficients  $\alpha_i^{(k)}$  is location-dependent, which means that the set of linear algebraic equations in Equation (2) need to solved for each location of interest at scale  $S_0$ .

The conditional covariance at scale  $S_0$  can be derived as

$${}^{(c)}C_Y^{(0)}(\mathbf{x}, \mathbf{y}) = C_Y^{(0)}(\mathbf{x}, \mathbf{y}) - \sum_{k=1}^K \sum_{i=1}^{N_k} \alpha_i^{(k)}(\mathbf{x}) C_Y^{(0,k)}(\mathbf{y}, \mathbf{x}_i^{(k)}), \quad (3)$$

where  $C_Y^{(0)}(\mathbf{x}, \mathbf{y})$  is the unconditional covariance between  $\mathbf{x}$  and  $\mathbf{y}$  at scale  $S_0$ , which in general is different from the unconditional covariance at other scales. The critical issue in this multiscale kriging method is how to find covariance functions within any scale and between different scales, which will be deliberated in the next section.

## Determination of Covariance between Different Scales

For convenience of presentation, we start from the one-dimensional problem. Given a second order stationary random field  $Y(x)$ , where  $x$  is a point in domain  $\Omega$ , we consider an averaged quantity of  $Y(x)$  over a segment of length  $T$  centered at  $x$ ,

$$Y_T(x) = \frac{1}{T} \int_{x-T/2}^{x+T/2} Y(u) du. \quad (4)$$

Since  $Y$  is a spatially random variable, and so is the averaged quantity  $Y_T$ . It is seen from the equation that  $Y_T$  has the same mean as the original variable  $Y$ , i.e.,  $\langle Y_T(x) \rangle = \langle Y(x) \rangle$ .

From Equation (4), one can derive the perturbation term as

$$Y'_T(x) = \frac{1}{T} \int_{x-T/2}^{x+T/2} Y'(u) du. \quad (5)$$

From this equation, it can be shown that the variance of  $Y_T$  is different from that of  $Y$  and can be written as  $\text{var}(Y_T(x)) = \sigma_Y^2 \gamma(T)$ , where  $\sigma_Y^2$  is the variance of  $Y$  and  $\gamma(T)$  is called the variance function [Vanmarcke,1983]. The variance function  $\gamma(T)$  measures the reduction of the point variance under local averaging and may be found as

$$\gamma(T) = \frac{1}{T^2} \int_0^T \int_0^T \rho(x_1 - x_2) dx_1 dx_2 = \frac{2}{T} \int_0^T \left(1 - \frac{\tau}{T}\right) \rho(\tau) d\tau. \quad (6)$$

where  $\rho$  is the correlation function of  $Y(x)$ . The variance function satisfies  $\gamma(T) \geq 0$ ,  $\gamma(0) = 1$ , and  $\gamma(-T) = \gamma(T)$ . Note that for a stationary field  $Y(x)$ ,  $Y_T(x)$  is also stationary. For a general form of covariance function  $\rho(\tau)$ ,  $\gamma(T)$  in Equation (6) should be evaluated numerically. However, for some special correlation functions,  $\gamma(T)$  can be derived analytically. For example, for an exponential correlation function  $\rho(\tau) = \exp(-|\tau|/\lambda)$ , where  $\lambda$  is the correlation length of  $Y(x)$ , we have

$$\gamma(T) = \gamma_1^e(T, \lambda) = 2 \left(\frac{\lambda}{T}\right)^2 \left(\frac{T}{\lambda} - 1 + e^{-T/\lambda}\right), \quad (7)$$

and for a Gaussian correlation function  $\rho(\tau) = \exp(-\tau^2/\lambda^2)$ ,

$$\gamma(T) = \gamma_1^g(T, \lambda) = \left(\frac{\lambda}{T}\right)^2 \left(\sqrt{\pi} \frac{T}{\lambda} E(T/\lambda) + e^{-T^2/\lambda^2} - 1\right), \quad (8)$$

where  $E$  is the error function. Subscript “1” in Equations (7) and (8) denotes variance functions for one-dimensional problems, and superscripts “e” and “g” stands for exponential and Gaussian covariance functions, respectively. Note that  $\gamma(T)$  satisfies  $\lim_{T \rightarrow \infty} \gamma(T) = 0$  for all these cases, which is the condition for ergodicity in the mean.

The covariance between two averaged random variables  $Y_T$  and  $Y_{T'}$ , where  $T$  and  $T'$  are two segments in the domain and may represent two different resolutions, can be expressed as [Vanmarcke, 1983]

$$\text{cov}(Y_T, Y_{T'}) = \frac{\sigma_Y^2}{2TT'} \sum_{k=0}^3 (-1)^k T_k^2 \gamma(T_k), \quad (9)$$

where  $T_k$  are defined in Figure 1. Although this figure depicts a special case in which  $T$  and  $T'$  are partially overlapping, Equation (9) is valid no matter whether they are overlapping or not. For a given correlation function  $\rho$ , once the variance function  $\gamma$  is found, one can compute  $\text{cov}(Y_T, Y_{T'})$  from Equation (9).

The above derivations can be easily extended to two-dimensional random fields. The local average of a field  $Y(\mathbf{x})$ , where  $\mathbf{x} = (x_1, x_2)$ , over a rectangular block  $A$  centered at  $\mathbf{x}$  is defined as

$$Y_A(\mathbf{x}) = \frac{1}{|A|} \int_A Y(\mathbf{y}) d\mathbf{y}, \quad (10)$$

where  $|A|$  denotes the area of the block  $A$ . The covariance function between any two blocks  $A$  and  $A'$ , which can be considered as two different resolutions, can be written as [Vanmarcke, 1983]

$$\text{cov}(Y_A, Y_{A'}) = \frac{\sigma_Y^2}{4|A||A'|} \sum_{k=0}^3 \sum_{m=0}^3 (-1)^{k+m} T_{1k}^2 T_{2m}^2 \gamma(T_{1k}, T_{2m}) \quad (11)$$

where  $T_{1k}$  and  $T_{2m}$  are defined in Figure 2 and the variance function  $\gamma$  is given as

$$\gamma(T_{1k}, T_{2m}) = \frac{4}{T_{1k} T_{2m}} \int_0^{T_{1k}} \int_0^{T_{2m}} \left(1 - \frac{\tau_1}{T_{1k}}\right) \left(1 - \frac{\tau_2}{T_{2m}}\right) \rho(\tau_1, \tau_2) d\tau_1 d\tau_2. \quad (12)$$

In particular, if the covariance of  $Y(\mathbf{x})$  is an exponential correlation function  $\rho(\tau_1, \tau_2) = \exp(-|\tau_1|/\lambda_1 - |\tau_2|/\lambda_2)$ , where  $\lambda_1$  and  $\lambda_2$  are the correlation lengths in  $x_1$  and  $x_2$  directions,

respectively, one has  $\gamma(T_{1k}, T_{2m}) = \gamma_1^e(T_{1k}, \lambda_1)\gamma_1^e(T_{2m}, \lambda_2)$ , and for an Gaussian correlation function  $\rho(\tau_1, \tau_2) = \exp(-\tau_1^2/\lambda_1^2 - \tau_2^2/\lambda_2^2)$ ,  $\gamma(T_{1k}, T_{2m}) = \gamma_1^g(T_{1k}, \lambda_1)\gamma_1^g(T_{2m}, \lambda_2)$ .

Similarly, for three-dimensional problems, the local average of the random field  $Y(\mathbf{x})$  is defined as

$$Y_V(\mathbf{x}) = \frac{1}{|V|} \int_V Y(\mathbf{y}) d\mathbf{y}, \quad (13)$$

where  $V$  is the block centered at  $\mathbf{x}$  and  $|V|$  is the volume of the block. The covariance between two blocks  $V$  and  $V'$  can be expressed as

$$\text{cov}(Y_V(\mathbf{x}), Y_{V'}(\mathbf{x}')) = \frac{\sigma_Y^2}{8|V||V'|} \sum_{k=0}^3 \sum_{m=0}^3 \sum_{n=0}^3 (-1)^{k+m+n} T_{1k}^2 T_{2m}^2 T_{3n}^2 \gamma(T_{1k}, T_{2m}, T_{3n}), \quad (14)$$

where  $|V|$  and  $|V'|$  stand for the volume of blocks  $V$  and  $V'$ , and  $T_{1k}$  and  $T_{2m}$ ,  $k, m = 1, 2, 3$ , are various lengths defined similarly as in the two-dimensional case, and the variance function  $\gamma$  is given as

$$\begin{aligned} \gamma(T_{1k}, T_{2m}, T_{3n}) &= \frac{8}{T_{1k} T_{2m} T_{3n}} \int_0^{T_{1k}} \int_0^{T_{2m}} \int_0^{T_{3n}} \left(1 - \frac{\tau_1}{T_{1k}}\right) \left(1 - \frac{\tau_2}{T_{2m}}\right) \left(1 - \frac{\tau_3}{T_{3n}}\right) \\ &\quad \rho(\tau_1, \tau_2, \tau_3) d\tau_1 d\tau_2 d\tau_3. \end{aligned} \quad (15)$$

If the covariance function is exponential correlation function  $\rho(\tau_1, \tau_2, \tau_3) = \exp(-|\tau_1|/\lambda_1 - |\tau_2|/\lambda_2 - |\tau_3|/\lambda_3)$ ,  $\gamma(T_{1k}, T_{2m}, T_{3n}) = \gamma_1^e(T_{1k}, \lambda_1)\gamma_1^e(T_{2m}, \lambda_2)\gamma_1^e(T_{3n}, \lambda_3)$ , and for the Gaussian correlation function  $\rho(\tau_1, \tau_2, \tau_3) = \exp(-\tau_1^2/\lambda_1^2 - \tau_2^2/\lambda_2^2 - \tau_3^2/\lambda_3^2)$ ,  $\gamma(T_{1k}, T_{2m}, T_{3n}) = \gamma_1^g(T_{1k}, \lambda_1)\gamma_1^g(T_{2m}, \lambda_2)\gamma_1^g(T_{3n}, \lambda_3)$ .

## Illustrative Examples

In this section, we use several synthetic examples to illustrate the proposed algorithm for estimating parameter fields at different scales by incorporating multiscale measurements. In each of these examples, we generate a random field at a finest scale, given statistics (mean, variance, and correlation lengths) of the field. By local averaging, we derive fields at different coarse scales, and then take a number of samples at different scales. Using these samples,

we estimate the kriged fields and their corresponding conditional covariance at different scales and compare these kriged fields to the “true” fields to assess the performance of the multiscale kriging method.

In the first example, we consider a one-dimensional column of length 256 (at any consistent unit), discretized into 256 grid of size 1. A random field with zero mean, unit variance, and separable, isotropic exponential covariance function of a correlation length 20 is generated at this grid, using the Karhunen-Loève decomposition method [Zhang and Lu, 2004]. This field is taken as the true field at this finest scale ( $S_1$ ). At any coarse scale, the true field is computed from the finest scale using Equation (4). We calculate the “true” fields at two coarse scales, at  $\Delta x = 2$  ( $S_2$ ) and  $\Delta x = 4$  ( $S_3$ ), which correspond to grids of 128 and 64, respectively. All these three “true” fields will be used to assess the accuracy of the kriged fields.

We then take  $N_1 = 16$  and  $N_3 = 4$  samples at scales  $S_1$  and  $S_3$ , respectively. The locations of these sample at the fine scale are indicated in Figure 3 as triangles along the horizontal axis, and the locations of coarse scale samples depicted the top of each diagram. There is no data at the intermediate scale  $S_2$ . Our purpose is to estimate the conditional mean and conditional covariance of the field at all three scales.

The estimated mean fields at three different scales are illustrated in Figure 3. Figure 3A compares the fine-scale true field (red curves) and the estimated field using the fine-scale measurements alone (green curves) as well as the estimated field using both coarse- and fine-scale measurements. It is seen from the figure that, although the estimate using the fine-scale measurements alone captures the general trend of the true field, incorporating coarse-scale measurements does improves the estimate locally. The range of influence of the coarse-scale measurements depends on the correlation length of the unconditional fields. In the regions that are far away from the coarse-scale measurements, these measurements do not have a significant impact on estimates. In addition, at this fine scale, the estimate using



multiscale measurements (blue curve) honors the fine scale measurements, but it does not honor the coarse-scale measurements. The estimation errors using different sets of data can be measured using the root-mean-squared error (RMSE). The RMSE is reduced from 0.746 for the kriged field using the fine-scale measurements only to 0.686 using both the fine- and coarse-scale measurements.

Figure 3B shows that at the coarse scale the kriged field (the green curve) using the coarse-scale measurements alone also captures the general trend of the field and honors the measurements at this scale, but it is relatively smooth and does not provide detailed variability of the field. By incorporating the fine-scale measurements, the estimate has been significantly improved (blue curve). The RMSE is reduced from 0.754 for the kriged field using the coarse-scale measurements alone to 0.601 using both the fine- and coarse-scale measurements. Note that the estimate at the coarse scale in general will not honor the fine-scale measurements.

It should be pointed out that, although the blue curves in Figures 3A and B are kriged fields using both coarse- and fine-scale measurements, these two fields differs slightly, because they represent the conditional mean fields at two different scales.

Figure 3C illustrates the kriging estimates using all measurements for the scale  $\Delta x = 2.0$ , at which there is no measurement at all. In general, both coarse- and fine-scale measurement are not honored at this scale. However, it is seen that the estimated field is reasonably close to the true field at this scale.

Figure 4 depicts the conditional variance of estimated fields at three different scales. At the fine scale, as shown in Figure 4A, using the measurements at this scale alone reduces the conditional variance significantly, especially near the measurement locations, where the conditional variance is zero. Conditional variance is further reduced once the coarse-scale measurements are taken into account. Although the conditional variance at the coarse-scale measurement locations has been significant reduced, the variance is not exactly zero, because

knowing a value at a location at the coarse-scale is not enough to infer the exact value at the same location at the fine scale. The same is true at the coarse scale, as illustrated in Figure 4B. At this coarse scale, the conditional variance at the fine-scale measurement locations is not zero, though it is very small. At scale  $S_2$  where there is no measurement available, the conditional variance is not zero at all coarse- or fine-scale measurement locations (Fig. 4C), but the conditional variance at this scale has been significantly reduced, as compared to the unconditional variance of  $\sigma_Y^2 = 0.951$  at this scale.

In the second case, we consider a two-dimensional domain of  $128 \times 128$ , discretized into  $1 \times 1$  elements (scale  $S_1$ , 16384 elements in total). A random field with zero mean, unit variance, and an isotropic separable exponential covariance function of correlation length  $\lambda = 20$  is generated using the Karhunen-Loève decomposition method [Zhang and Lu, 2004]. From this field, two additional fields of grids 64 (scale  $S_2$ ,  $\Delta x = \Delta y = 2$ , 4096 elements) and 32 (scale  $S_3$ ,  $\Delta x = \Delta y = 4$ , 1024 elements) are derived using Equation (10). These three fields are considered as “true” fields. Suppose that  $N_1 = 50$  measurements are taken from fine scale  $S_1$ ,  $N_3 = 10$  measurements from coarse scale  $S_3$ , and no observation is available at the intermediate scale  $S_2$ . The locations of these measurements are displayed in Figure 5.

Figure 6 compares the true field at the finest scale (Fig. 6A) with the kriged field using the fine-scale measurements alone (Fig. 6B) and the kriged field using measurements at both fine and coarse scales (Fig. 6C). The figure shows that the kriged field using the fine-scale measurements alone captures the most of the heterogeneities of the true field but additional measurements in the coarse scale improves the accuracy of the estimated field slightly. The root mean square error of the kriged fields is reduced from 0.750 for the estimated field using the fine-scale measurements to 0.684 for the field estimated using measurements at both the fine and coarse scales.

Figure 7 illustrates the comparison between the fields of the conditional variance at the fine scale, conditioned at fine-scale measurements only (Fig. 7A) and at both fine-

and coarse-scale measurements (Fig. 7B). A significant reduction of the local conditional variance is evident around the coarse-scale conditioning points by incorporating coarse-scale measurements in estimating the fine-scale field.

At the coarse scale, since only a small number of measurements are available, the kriged field using these coarse-scale measurements alone is very close to a relatively homogeneous, unconditional mean field, as illustrated in Figure 8B. However, if the fine-scale measurements are also incorporated into the kriged field, it becomes much close to the true field (Fig. 8C). The root mean square error of the kriged fields at the coarse scale is reduced from 0.865 for the estimated field using the coarse-scale measurements to 0.619 for the field estimated using measurements at both the fine and coarse scales.

It should be noted that the fields presented in Figures 6C and 8C are slightly different, even though both of them are kriged fields using all fine- and coarse-scale measurements. These two fields represent conditional fields at two different scales.

Figure 9 compares the conditional variance at the coarse scale, using coarse-scale measurements alone (Fig. 9A) and using all coarse- and fine-scale measurements (Fig. 9B). The figure demonstrates that incorporating fine-scale measurements significantly reduces the conditional variance at the coarse scale.

At the intermediate scale, where there is no data available, the conditional mean and variance can be estimated from measurements at other scales. Figure 10 compares the true field at this scale (Fig. 10A) against the estimated conditional mean field using measurements at both fine and coarse scales (Fig. 10B). Figure 11 illustrates the conditional variance at this intermediate scale by using measurements at other two scales. It is seen from these figures that the conditional mean field estimated using measurements at other scales is close to the true field and that the conditional variance can be significantly reduced. This example demonstrates that this multiscale simple kriging method can be used to estimate the conditional mean and variance fields at any scale where there is no data available, as

long as measurements are available at some other scales.

## 1 Summary and Conclusions

In this study, we propose a simple kriging algorithm to incorporate data observed at multi-scales (multi-resolutions). We assume that there are a number of measurements at different scales that may be different from the target scale at which the parameter values are needed. Similar to the simple kriging, the parameter at the target scale is represented as a linear combination of all available measurements and the coefficients in this linear combination are solved from the kriging system that is related to covariance functions across the scales. The key point in this method is to find the covariance functions between blocks at different scales. We illustrated the method using several one-dimensional and two-dimensional synthetic examples.

These examples demonstrate that, at any scale at which some measurements are available, by incorporating measurements from all scales, the estimated field is better than the field estimated only using the measurements at this scale.

Second, if measurements are available at the target scale, these measurements will be honored. However, measurements at other scales will not be honored at the target scale, even though they will reduce the conditional covariance at the target scale.

Furthermore, This method also allow us to estimate a parameter field at the scale that does not have any measurements. In this case, the conditional mean field and conditional covariance can be found using measurements at other scales. Of course, all measurements will not be honored at the target scale. The method may be useful in some applications, such as numerical adaptive mesh refinement.

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## Figure Captions

**Figure 1** Schematic diagram defining various distances characterizing the relative positions of two segments.

**Figure 2** Schematic diagram defining various distances characterizing the relative positions of two rectangular blocks.

**Figure 3** Comparison of the one-dimensional true fields and kriged mean fields at three scales: (A) fine scale, (B) coarse scale, and (C) the intermediate scale at which no measurements are available.

**Figure 4** Comparison of the conditional variance for the one-dimensional case computed using different sets of data at three scales: (A) fine scale, (B) coarse scale, and (C) the intermediate scale at which no measurements are available.

**Figure 5** Locations of conditioning points in the two dimensional example with  $N_1 = 50$  (circles) and  $N_3 = 10$  (squares).

**Figure 6** Comparison of the true field (A), and the kriged mean fields using fine-scale data (B) and multiscale data (C), at the two-dimensional fine scale.

**Figure 7** Conditional variance at the fine scale, computed using fine-scale data only (A), and multiscale data (B).

**Figure 8** Comparison of the true field (A), and the kriged mean fields using fine-scale data (B) and multiscale data (C), at the coarse scale.

**Figure 9** Conditional variance at the coarse scale, computed using fine-scale data only (A), and multiscale data (B).

**Figure 10** Comparison of the true field (A), and the kriged field using multiscale data (B), at the intermediate scale where no measurements are available.

**Figure 11** Conditional variance at the intermediate scale using multiscale data.

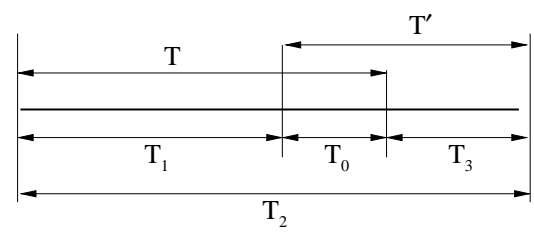


Figure 1:



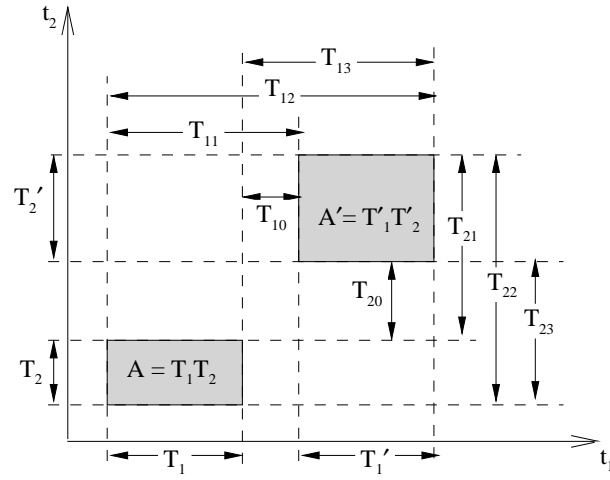


Figure 2:

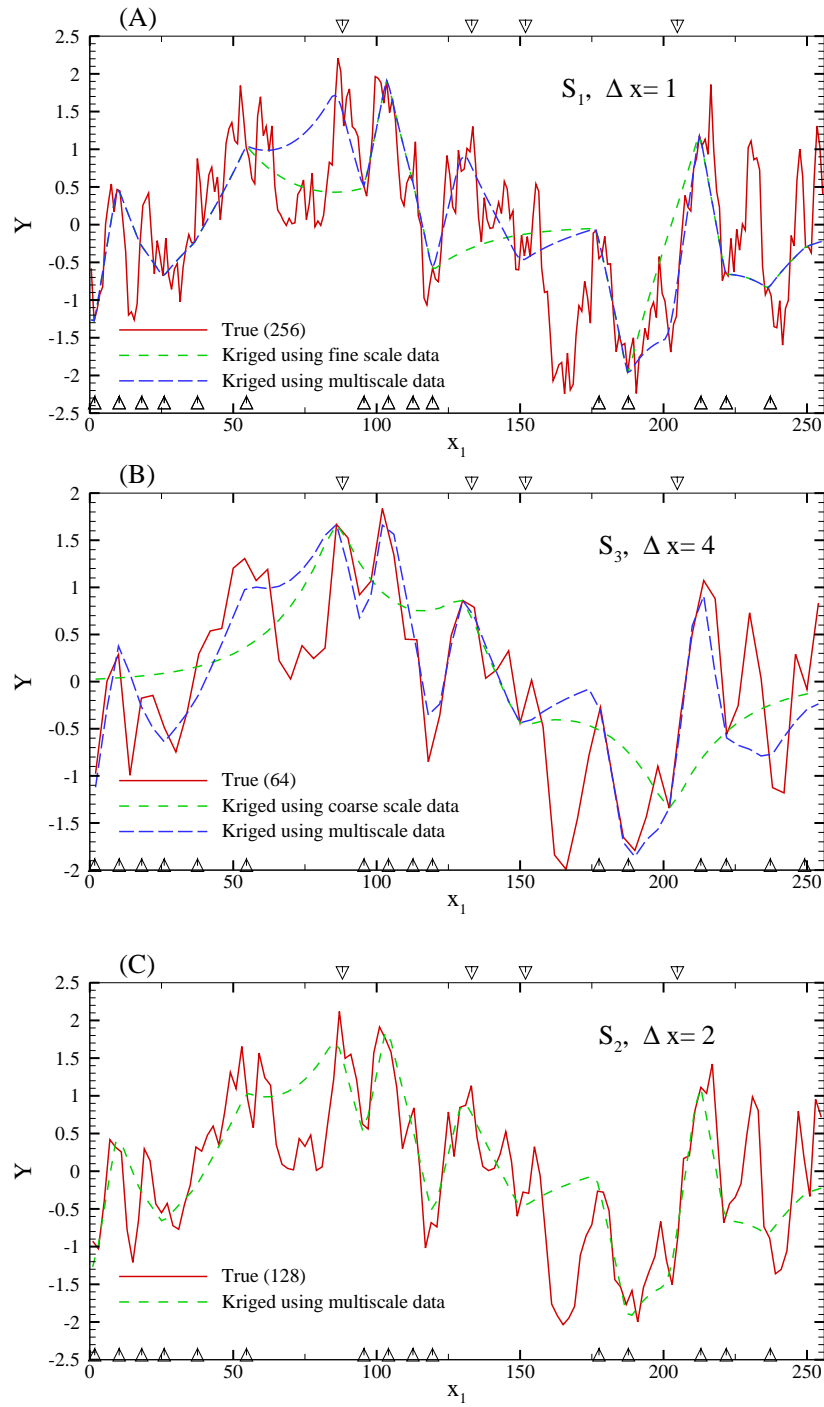


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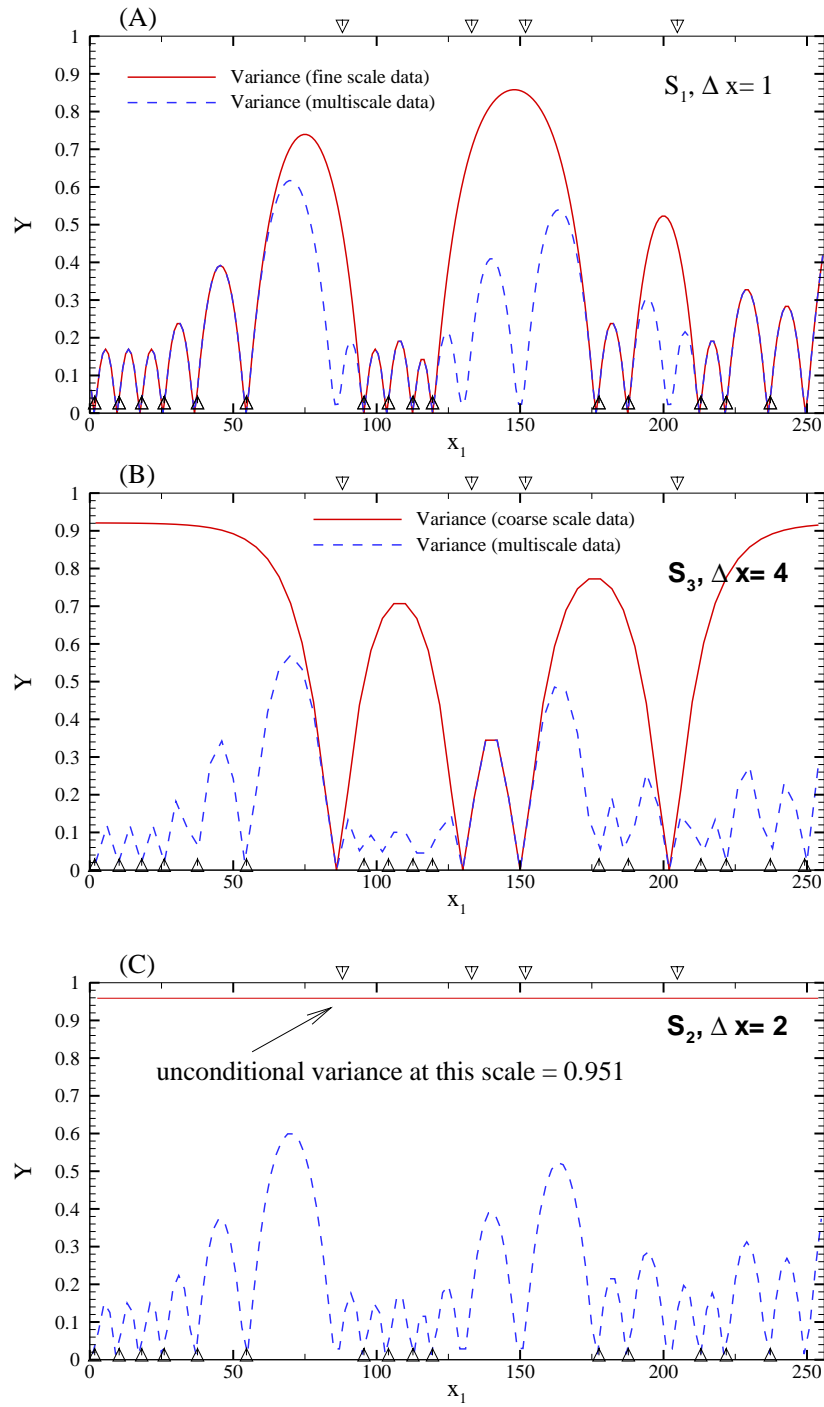


Figure 4:

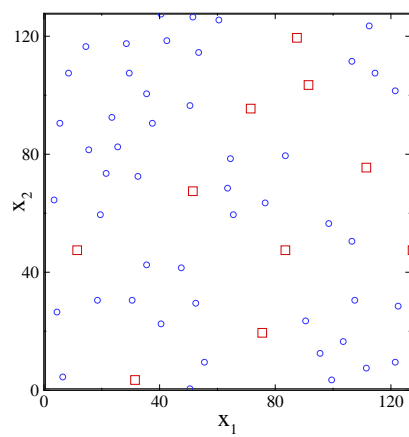


Figure 5:

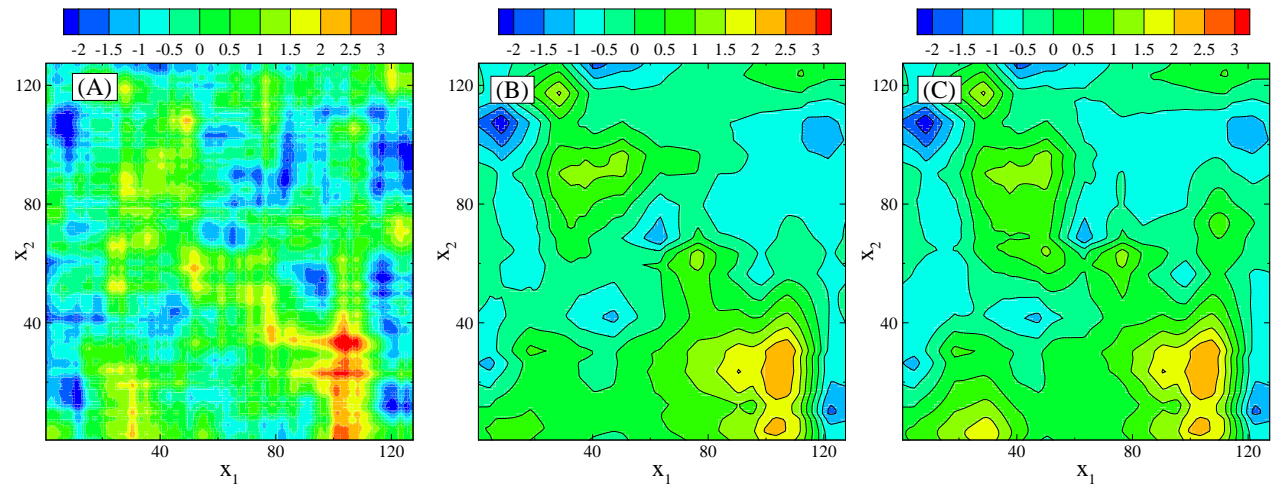


Figure 6:

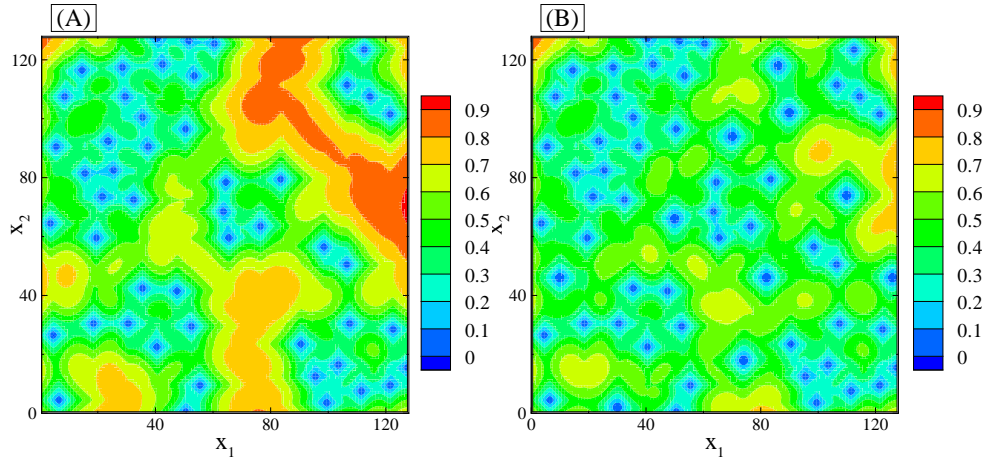


Figure 7:

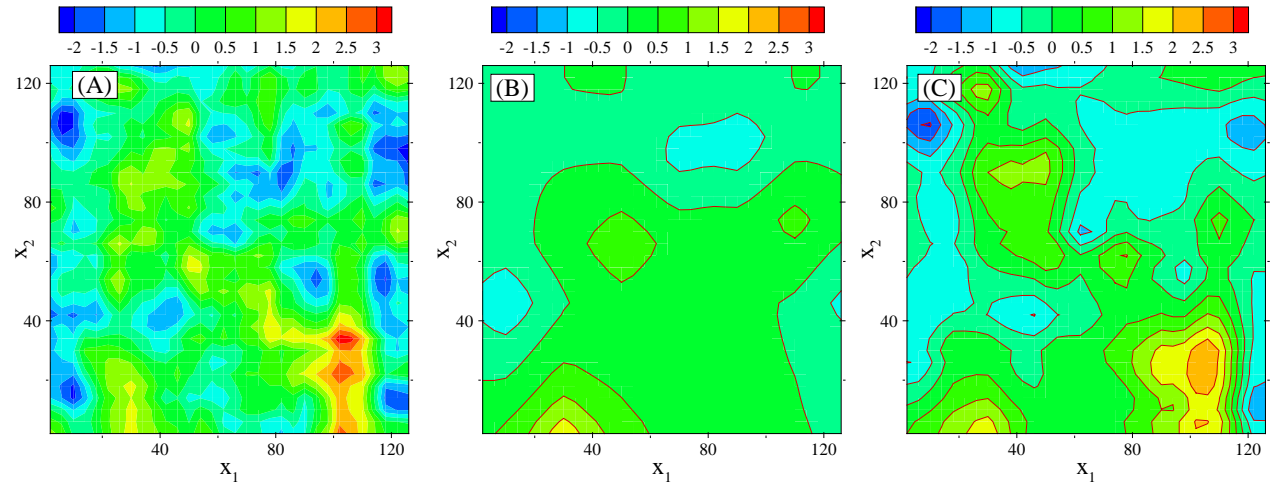


Figure 8:

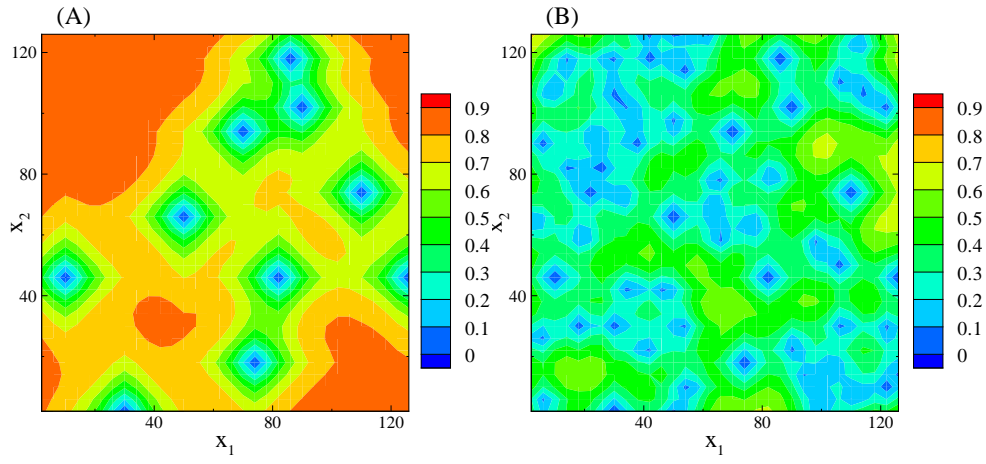


Figure 9:



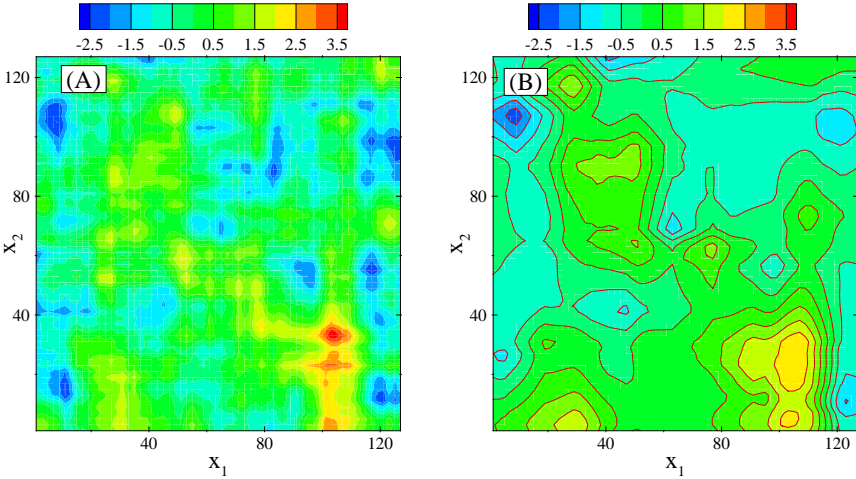


Figure 10:

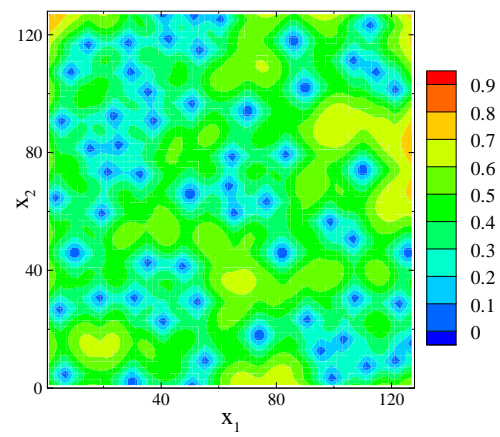


Figure 11: